

Monte Carlo study of lipid bilayers and their interactions with polymer chains

Jens-Uwe Sommer¹, Marco Werner²

¹Leibniz-Institut für Polymerforschung Dresden – sommer@ipfdd.de

²Leibniz-Institut für Polymerforschung Dresden – werner-marco@ipfdd.de

Abstract

We apply the Bond Fluctuation Method to simulate static and dynamic properties of lipid bilayers and their interactions with polymers using an explicit solvent model. The latter allows us to simulate strong hydrophobic effects. Our model is used to simulate self-assembled planar bilayers as well as vesicles efficiently on a coarse grained level, where we focus on the interaction between membranes and single polymer chains. By changing the hydrophobicity of the polymer chains a transition from the non-adsorbed state of the chains into the strongly adsorbed state can be observed. In the latter case the hydrophobic chain is embedded and trapped into the hydrophobic layer of the membrane. For intermediate hydrophobicities the chains are in a transition state where they are able to pass spontaneously through the membrane. Here, the state of the lipid membrane close to the chain is highly disturbed. At the transition state, which might be associated with an adsorption transition of polymer chains at a potential trap, we also observe a maximum of the permeability of the membrane with respect to solvent molecules. We analyze the transition state using several local static and dynamic properties of the membrane and of the chain.

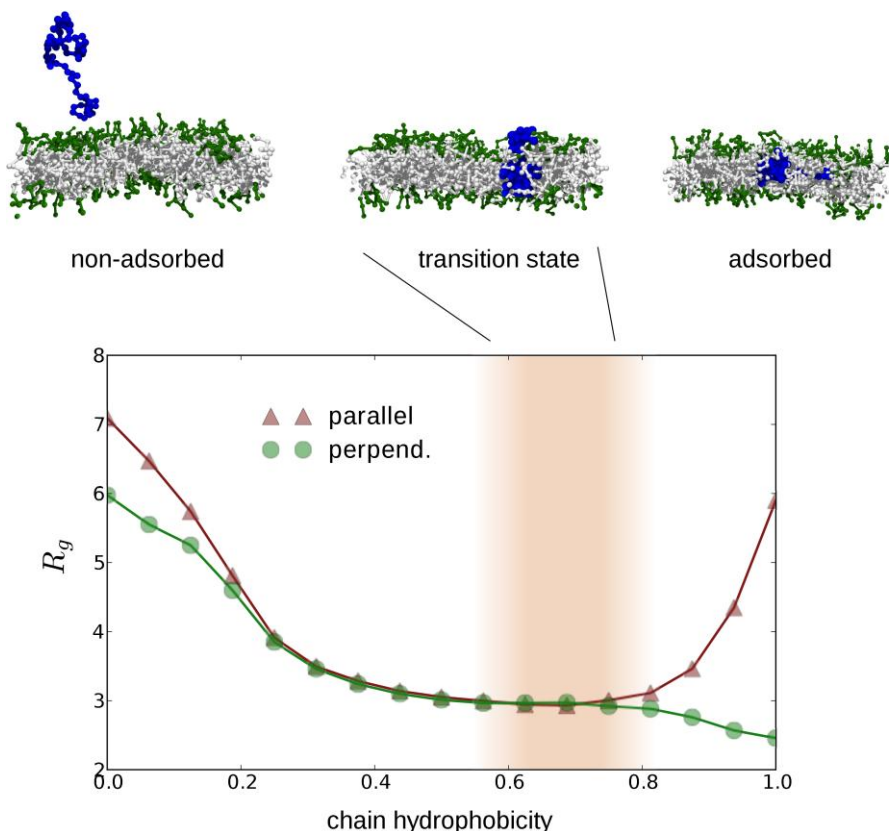


Fig. 1

. Simulation results for the components of the radius of gyration of a polymer chain parallel and perpendicular to a lipid bilayer depending on the chain hydrophobicity relative to the hydrophobicity of the lipid-tails.